5,5-Dimethyl-1-ethyl-1,3-cyclopentadiene

Inchi: InChI=1S/C9H14/c1-4-8-6-5-7-9(8,2)3/h5-7H,4H2,1-3H3
InchiKey: BMLYRJOYQDJMOR-UHFFFAOYSA-N
Formula: C9H14
SMILES: CCC1=CC=CC1(C)C
Mol. weight [g/mol]: 122.21

Physical Properties

Property code	Value	Unit	Source
gf	106.25	kJ/mol	Joback Method
hf	-49.28	kJ/mol	Joback Method
hfus	8.76	kJ/mol	Joback Method
hvap	35.98	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
ripol	1225.00		NIST Webbook
ripol	1225.00		NIST Webbook
tb	424.14	K	Joback Method
tc	629.50	K	Joback Method
tf	240.03	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.21	J/mol×K	424.14	Joback Method
cpg	246.37	J/mol×K	458.37	Joback Method
cpg	260.44	J/mol×K	492.59	Joback Method
cpg	273.54	J/mol×K	526.82	Joback Method
cpg	285.76	J/mol×K	561.05	Joback Method
cpg	297.20	J/mol×K	595.27	Joback Method
cpg	307.96	J/mol×K	629.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R618414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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